SMMC studies of $N = Z$ pf-shell nuclei with pairing-plus-quadrupole Hamiltonian

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(February 3, 2008)

Abstract

We perform Shell Model Monte Carlo calculations of selected $N = Z$ pf-shell nuclei with a schematic hamiltonian containing isovector pairing and quadrupole-quadrupole interactions. Compared to realistic interactions, this hamiltonian does not give rise to the SMMC "sign problem", while at the same time resembles essential features of the realistic interactions. We study pairing correlations in the ground states of $N = Z$ nuclei and investigate the thermal dependence of selected observables for the odd-odd nucleus ^{54}Co and the even-even nuclei ^{60}Zn and ^{60}Ni. Comparison of the present results to those with the realistic KB3 interaction indicates a transition with increasing temperature from a phase of isovector pairing dominance to one where isoscalar pairing correlations dominate. In addition, our results confirm the qualitative reliability of the procedure used to cure the sign problem in the SMMC calculations with realistic forces.

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I. INTRODUCTION

Motivated by fundamental nuclear structure questions and by astrophysical applications, the study of extremely neutron- and proton-rich nuclei is currently at the forefront of research interests in nuclear physics. Novel proton-rich radioactive ion-beam facilities offer the possibility of exploring the structure of nearly self-conjugate ($N \sim Z$) nuclei in the medium mass range $Z \lesssim 50$. i A focus of interest will be the proton-neutron (pn) interaction, which has long been recognized to play an important role in $N = Z$ nuclei (see Ref. [1] for an early review). Of particular relevance in self-conjugate odd-odd nuclei in the pf shell should be the pn isovector correlations as it is evident from the ground state spins and isospins. While the sd-shell odd-odd $N = Z$ nuclei (with the exception of ^{34}Cl) have ground states with isospin $T = 0$ and angular momenta $J > 0$, self-conjugate odd-odd $N = Z$ nuclei in the pf shell ($A > 40$) have ground states with $T = 1$ and $J^\pi = 0^+$ (the only known exception is ^{58}Cu) indicating the dominance of isovector pn pairing. In addition, in ^{74}Rb the ground state isospin is also $T = 1$ [2], again arising from isovector pn correlations.

Early studies of isovector and isoscalar pn pairing for sd-shell nuclei [3] and for nuclei at the beginning of the pf-shell [4] used the Hartree-Fock-Bogoliubov (HFB) formalism. Their conclusion [1] that the $T = 1$ pn pairing is unimportant is surprising since, as pointed out above, the $T = 1$ ground state isospin of most odd-odd $N = Z$ nuclei with $A \geq 40$ clearly points to the role of $T = 1$ pn pairing in these nuclei.

Although HFB calculations have pioneered the study of pairing in $N = Z$ nuclei, the method of choice to study pair correlations is the interacting shell model. Within the sd shell [5] and at the beginning of the pf-shell [6,7] the interacting shell model has proven to give an excellent description of all nuclei, including the correct reproduction of the spin-isospin assignments of self-conjugate $N = Z$ nuclei. However, the conventional shell model using diagonalization techniques is currently restricted to nuclei with masses $A \leq 50$ due to computational limitations. These limitations are overcome by the Shell Model Monte Carlo (SMMC) approach [8,9]. Using this novel method, it has been demonstrated [10] that complete pf shell calculations using the modified Kuo-Brown interaction well reproduce the ground state properties of even-even $N = Z$ nuclei with $A \leq 60$. Additionally the SMMC approach naturally allows the study of thermal properties.

In this paper we use the SMMC method. However, instead of the realistic nucleon-nucleon interaction we use a simplified interaction containing only the isovector pairing interaction and the quadrupole-quadrupole force. Such interaction is nevertheless able to reproduce semi-quantitatively the essential features of nuclear structure such as the pairing gaps and B($E2$) values [11]. At the same time such a hamiltonian does not give rise to the "sign problem" which with the realistic interaction can be overcome only by the "g-extrapolation" [12]. The present calculations, therefore, serve a dual purpose. On one hand, they represent a test of the "g-extrapolation" as far as main nuclear properties are concerned. At the same time, they allow us to draw important conclusion with much more modest computational effort and without inducing potential systematic errors.

II. MODEL

The SMMC approach was developed in Refs. [8,9], where the reader can find a detailed description of the ideas underlying the method, its formulation, and numerical realization. As the present calculations follow the formalism developed and published previously, a very brief description of the SMMC approach suffices here. A comprehensive review of the SMMC method and its applications can be found in Ref. [13].

The SMMC method describes the nucleus by a canonical ensemble at temperature $T = \beta^{-1}$ and employs a Hubbard-Stratonovich linearization [14] of the imaginary-time many-body propagator, $e^{-\beta H}$, to express observables as path integrals of one-body propagators in fluctuating auxiliary fields [8,9]. Since Monte Carlo techniques avoid an explicit enumeration of the many-body states, they can be used in model spaces far larger than those accessible to conventional methods. The results are in principle exact and are in practice subject only to controllable sampling and discretization errors. However, SMMC studies with "realistic interactions" are hampered by potential systematic uncertainties introduced by the infamous sign-problem [15]. These problems are avoided, and the SMMC is in fact an exact solution to the many-body shell model problem, if a Hamiltonian of the form pairing+multipole-multipole interaction is used [9]. The schematic hamiltonian we use in the present work is of this form

$$H = \sum_{jmt_z} \epsilon(j) a^\dagger_{jmt_z} a_{jmt_z} - G/4 \sum_{jj't_z} A^{T=1t_z\dagger}_{JM=00} A^{T=1t_z}_{JM=00} - \chi \sum_\mu (-1)^\mu Q_\mu Q_{-\mu} \ , \tag{1}$$

where Q_μ is the mass quadrupole moment operator with projection μ, $a^\dagger_{jmt_z}$ creates a nucleon of isospin projection t_z in the orbital jm, and the two particle creation operator $A^\dagger$ is defined below.

The summation over the single particle energies is restricted to the four states in the pf shell. The single particle energies are taken from the original Kuo-Brown interaction KB3 [16]. We use the pairing constant $G = 20/A$ MeV from [11]. In calculating the ground state properties we cool the nuclei to $T = 0.25$ MeV. Experience shows that this is usually sufficient to have only minimal thermal admixtures of excited states.

In order to measure the overall pair correlations in nuclear wave functions, we use the BCS pair operator (for $T = 1, JM = 00$)

$$\Delta^{Tt_z\,\dagger}_{JM} = \sum_\alpha A^{Tt_z\dagger}_{JM}(\alpha) \ , \ \ A^{Tt_z\dagger}_{JM}(\alpha) = [a^\dagger_a a^\dagger_b]^{Tt_z}_{JM}, \tag{2}$$

where α is an index combining the single particle labels a and b. The quantity

$$\mathcal{N}_{t_z} = \sum_M \langle \Delta^{Tt_z\dagger}_{JM} \Delta^{Tt_z}_{JM} \rangle \tag{3}$$

is then a measure of the strength of pair correlations with isospin projection t_z, or in other words, of the number of nucleon pairs with the angular momentum J and isospin and its projection Tt_z. In the following we will restrict ourselves to isovector s-wave pairing ($J = 0$), which, however, plays the most important role in the low-energy spectrum of the nuclei of interest in this work. Earlier SMMC results for BCS pairing in nuclei in the mass range

$A = 48 - 60$ obtained with the "realistic" KB3 interaction [16] and involving therefore the g-extrapolation are published in Refs. [10,13,17,18].

We still have to fix the coupling constant χ of the quadrupole force. Compared with the original parametrization $\chi = 240/(b^4 A^{5/3})$ MeV/fm^4 (b is the oscillator length unit) as suggested in Ref. [11] we have rescaled the strength of the quadrupole-quadrupole interaction by a factor 0.6. The rescaled interaction then gives approximately the same results for $\langle Q_p^2 \rangle$, $\langle Q_n^2 \rangle$, and $\langle (Q_p + Q_n)^2 \rangle$ ($Q_{p(n)}$ is the proton (neutron) quadrupole operator) as the realistic KB3 interaction [16]. The latter has been demonstrated to give a good description of $B(E2)$ strength in the mass range $A = 48 - 60$ [7,10]. Unlike in the original application of the pairing plus quadrupole hamiltonian [11], we use now a pairing interaction which is isospin symmetric, i.e. we have replaced the like-particle-only pairing (nn and pp) by the general isovector one.

III. RESULTS

In Fig. 1 we show the BCS pairing strengths $\mathcal{N}_{t_z}$, eq. (3), for $pp = nn$ ($t_z = \pm 1$) and pn ($t_z = 0$) correlations in the ground states of $N = Z$ nuclei. Generally the schematic hamiltonian yields similar but slightly larger isovector correlations than the realistic hamiltonian (the results for that interaction are taken from [17,18]) as also seen in Fig. 1.

As a striking feature Fig. 1 shows a strong staggering in both the pp and pn pairing strengths when comparing neighboring even-even and odd-odd self-conjugate nuclei. In the latter, the isovector pn pairing clearly dominates the pp (and the identical nn) pairing and is always significantly larger than in the neighboring even-even $N = Z$ nuclei. In contrast, the like-nucleon pairing is noticeably reduced in the odd-odd nuclei relative to the values in the neighboring even-even nuclei. As pointed out by Engel et al. [18] the increased strength in pn pairing caused by the extra isovector proton-neutron pair appears to be a salient feature in odd-odd $N = Z$ nuclei with ground state isospin $T = 1$.

As an added bonus, we also note that the good agreement of the SMMC pairing results with the realistic KB3 interaction and with the schematic hamiltonian gives confidence in the g-extrapolation required in the SMMC calculations with the KB3 interaction due to the "sign problem".

As is obvious from Fig. 1, and has already been stressed elsewhere (e.g. [17,18]), odd-odd $N = Z$ nuclei are the ideal place to study isovector pn pairing correlations. We have used the self-conjugate odd-odd nucleus ^{58}Cu as a first example to explore some of the physics present in our model. To develop an understanding of the relative importance of the two parts of the interaction on the results, we have calculated several observables as a function of the pairing strength where we have scaled the coupling constant G of the pairing interaction in the hamiltonian by a factor λ. In Fig. 2 we show how the pn and pp pairing depends on the quantity λG. Obviously both pp and pn correlations increase with increasing λ, reaching saturation at about $\lambda = 3$. For all positive λ isovector pn correlations clearly dominate over pp or nn pairing. At $\lambda = 0$ the pairing correlations, using our definition, do not vanish since they get a contribution from the mean field and from the quadrupole force. Associated with the change in pair correlations, the isospin expectation value, shown in Fig. 3, increases rapidly from $\langle T^2 \rangle = 0.58$ at $\lambda = 0$ to $\langle T^2 \rangle \approx 2$ for $\lambda \geq 1$. In the same λ interval the angular

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momentum, also shown in Fig. 3, drops from $\langle J^2 \rangle = 8$ to $\langle J^2 \rangle = 2$ (The angular momentum is not strictly zero even for large λ since at the finite temperature $T = 0.25$ MeV, used in the present calculation in lieu of $T = 0$, excited states with $\langle J^2 \rangle > 0$ are slightly mixed into the expectation values).

The importance of the quadrupole interaction on the results are only minor. To see this, the results at $\lambda = 0$ in Figs. 2-3 should be compared with the ones without interaction (which we will call "mean-field results"). We find $\langle J^2 \rangle = 8.5$, $\langle T^2 \rangle = 0.8$, $\mathcal{N}_0 = 4.1$ and $\mathcal{N}_1 = 4.0$ on the mean-field level. Thus the quadrupole interaction has only noticeable influence on the isospin which it shifts towards $T = 0$.

In Fig. 4 we show the ground state energy expectation values for the $N = Z$ nuclei. The odd-odd nuclei are slightly less bound than the neighboring even-even nuclei. The displacement is approximately 1.1 MeV, and shows that the model with isovector pairing nevertheless accounts for the usual pairing displacement between the odd-odd and even-even nuclei. However, the calculated displacement is only about half of the experimental one. The discrepancy reflects the schematic nature of our hamiltonian; it might be related to the lack of isoscalar pn interaction.

Engel *et al.* [18] have shown that within an isotope chain with neutron (or proton) excess proton-neutron pairing is reduced, while the pairing among protons and among neutrons is increased. This result agrees with our findings, as is demonstrated in Fig. 5 using the nickel isotopes as an example. In the even-even $N = Z$ nucleus ^{56}Ni with neutron number $N = 28$ pp, nn, and pn pairing is identical. Clearly pn correlations drop drastically with either proton or neutron excess, while pp and nn pairing increases. The turn-over in nn pairing for $N < 26$ is simply caused by the approach to the empty neutron shell at $N = 20$, which also affects the pn pairing. We also show in Fig. 5 the average pairing (i.e. one third of the total pairing energy) for the series of nickel isotopes. Unlike its components, the total pairing energy is quite smooth, it depends only weakly on $N - Z$.

We now turn to the discussion of the thermal dependence of various observables. In Refs. [10,15,17] SMMC studies of the thermal dependence of selected observables have been presented for several even-even nuclei (including the $N = Z$ nucleus ^{52}Fe) and the odd-odd $N = Z$ nucleus ^{50}Mn. All these calculations had been performed with the KB3 interaction. As expected, a large excess of $J = 0^+$ like-particle pairing had been found in the ground states of the even-even nuclei with neutron excess. With increasing temperature, these pairing correlations decrease and at around $T = 1$ MeV the like-particle pairs break in these nuclei. In the even-even $N = Z$ nucleus ^{52}Fe an (approximate) isospin symmetry results in nearly identical pp, nn, and pn pairing; the pairs in all three isovector channels break at around $T = 1$ MeV. The thermal dependence of odd-odd $N = Z$ nuclei is different. The pn correlations, which dominate the ground state of the odd-odd $N = Z$ nuclei, decrease rapidly with temperature, while the like-particle pairing remains roughly constant to $T \approx 1.1$ MeV.

In order to elucidate these features further, we have performed SMMC calculations with the schematic hamiltonian for the even-even $N = Z$ nucleus ^{60}Zn and for the odd-odd $N = Z$ nucleus ^{54}Co. These studies are aimed at verifying the g-extrapolation required in the previous SMMC studies and at testing which of the essential physics observed in the temperature dependence of the pair correlations and of selected observables is already reproduced by the schematic pairing plus quadrupole hamiltonian. The SMMC calculations

have been performed for the temperature range 0.25 MeV to 5 MeV.

In Figs. 6-9 we show the temperature dependence of the expectation values of the energy, the isovector pair correlations, the isospin and the angular momentum for ^{54}Co and ^{60}Zn. The energy expectation value $\langle H \rangle$, shown in Fig. 6, increases, as required by general thermodynamic principles, with temperature, and it does so roughly linearly in the interval $T = 0.5 - 2$ MeV. For the even-even ^{60}Zn, like in ^{52}Fe studied earlier with the KB3 interaction, the energy expectation value increases very slowly at low temperatures ($T < 0.5$ MeV). This low-temperature behavior is well known and is related to the fact that in even-even nuclei the isovector pairing gap has to be overcome. Correspondingly, the heat capacity $C(T) = d\langle H \rangle/dT$ shows a significant excess over the mean-field values for temperatures $T = 0.6 - 1.4$ MeV, with the largest excess at around $T = 1$ MeV where the $J = 0^+$ pairs break. At higher temperatures $C(T)$ becomes negative in both nuclei as the finite model space requires $\langle H \rangle$ to approach a constant value in the high temperature limit.

The pair correlations are shown in two panels in Fig. 7. Like in the calculation with the KB3 interaction, the proton-neutron correlations in the odd-odd ^{54}Co decrease very rapidly with temperature for $T < 1$ MeV, while the like-particle correlations remain about constant in this temperature interval. At higher temperatures, $T > 1$ MeV, the isovector correlations slowly vanish, but remain larger than the mean-field values even up to temperatures $T = 5$ MeV. The behavior of pairing correlations in the even-even nucleus ^{60}Zn is rather different. The pn and like-particle correlations remain essentially identical at all temperatures.

Can one understand why the thermal dependence of the pairing strength is so different in the odd-odd and even-even $N = Z$ nuclei? The difference is explained by the uniqueness of the isospin properties of the odd-odd $N = Z$ nuclei. These nuclei are the only ones where states of different isospin, $T = 1$ and $T = 0$, are found close to each other at low excitation energies. In ^{54}Co the ground state is $T = 1$ with $T_Z = 0$ and $J^\pi = 0^+$. As explained above in that state the pn pair correlations dominate, and the like-particle correlations are reduced. However, at relatively low excitation energy one finds in these nuclei a multiplet of $T = 0$ states. Such states have necessarily nonvanishing angular momenta, and thus contribute efficiently to the corresponding thermal average. On the other hand, from isospin symmetry it follows that in the $T = 0$ states all three pairing strength $\mathcal{N}_{t_z}$ must be equal. Hence, at temperatures where the $T = 0$ states dominate the thermal average, the pn pair correlations are substantially reduced when compared to their ground state values, and the like-particle pairing correlations are somewhat enhanced, as seen in Fig. 7. This behavior is not restricted to the cases studied; it is quite generic and should be present in all odd-odd $N = Z$ nuclei with ground state isospin $T = 1$. In the sd shell the $T = 1$ state is usually an excited state at a low excitation energy. Thus its weight in a thermal average is strongly reduced compared to the pf shell nuclei. Consequently, there will be no dominance of pn correlations at low temperatures in odd-odd $N = Z$ nuclei in the sd shell.

The dependence of the isospin expectation value $\langle T^2 \rangle$ on temperature is also different in the odd-odd and even-even nuclei as seen in Fig. 8. While the isospin steadily increases in the even-even ^{60}Zn, it decreases first from its initial value of 2 (corresponding to $T = 1$) as the low-lying isospin $T = 0$ states become populated. The effect of the isovector pairing is clearly visible in a comparison with the mean-field values (obtained with the two-body interaction switched off). At low temperatures $T \leq 0.5$ MeV the isovector pair condensate results in the total isospin $T = 1$ in the odd-odd nucleus, while in the even-even the isovector

condensate makes total isospin $T = 0$. At higher temperatures ($T > 1.5$ MeV) both nuclei behave more or less similarly. An SMMC calculation with the KB3 interaction showed that isoscalar correlations, missing in our schematic Hamiltonian, reduce the isospin to nearly $\langle T^2 \rangle = 0$ at temperatures around 1 MeV in odd-odd nuclei.

The angular momentum expectation value $\langle J^2 \rangle$, shown in Fig. 9, increases rapidly with temperature from $\langle J^2 \rangle = 0$ at $T < 0.25$ MeV. Again, the presence of states with both isospins $T = 1$ and 0 in ^{54}Co and the pairing gap in ^{60}Zn causes more rapid increase of angular momentum in the odd-odd ^{54}Co than in the even-even ^{60}Zn.

Another aspect of the same phenomenon is the behavior of the level density parameter

$$a = \frac{\mathrm{d}\langle H \rangle}{\mathrm{d}T} / 2T \; . \tag{4}$$

The rapid decrease in pn correlations in the odd-odd nucleus generates an excess of levels, i.e. an increase in a (over the mean field) at lower temperatures than in the even-even nucleus where there is a strong pairing gap in all three isovector pairing channels. At higher temperatures, when the isovector pairs break, the even-even nuclei experience therefore more noticeable increase of the level density, with an increase in a over the mean-field value of about 1.5/MeV for ^{60}Zn and of about 1/MeV in ^{54}Co at $T = 1$ MeV. This behavior of the level density is therefore linked to the difference in the way the isovector pn and the like-particle correlations behave in these two systems as discussed above.

For realistic interactions the sign-problem is reduced with increasing temperature making direct SMMC calculations feasible without invoking the "g-extrapolation" procedure. We have performed such SMMC calculations for the KB3 interaction at $T \geq 2.5$ MeV. The results obtained for the isovector pair correlations and for $\langle J^2 \rangle$ are identical to those of our schematic Hamiltonian, confirming again that this interaction indeed describes these quantities very well. However, for both nuclei ^{54}Co and ^{60}Zn the isospin expectation values are significantly lower than for the schematic Hamiltonian (see Fig. 8). The origin of the different behavior are the isoscalar pn correlations, which are missing in the schematic Hamiltonian. As has been shown previously, the isoscalar pn correlations decrease less rapidly with increasing temperature than the isovector correlations and compete with the latter at moderate temperatures (say $T \geq 1.5$ MeV). These isoscalar correlations lower the energies of states with isospin $T = 0$ compared to calculations where these correlations are missing. Hence the isospin expectation value is smaller at moderate temperatures if the isoscalar correlations are included. To estimate the importance of isovector versus isoscalar correlations at these high temperatures we refer to the two following observations. First, by comparing $\langle T^2 \rangle$ for the realistic KB3 interaction and for the schematic Hamiltonian we find a reduction by more than a factor of two due to isoscalar correlations, while the schematic Hamiltonian gives results which are only about 10% lower than the mean-field values. Second, the isospin expectation values calculated with the KB3 interaction are nearly the same for the odd-odd and even-even $N = Z$ nuclei, in contrast to the marked differences between odd-odd and even-even $N = Z$ nuclei at low temperatures induced by the dominating isovector pairing, as discussed above. We conclude that at moderate temperatures the $N = Z$ nuclei are dominated by isoscalar correlations and that there is a transition from isovector to isoscalar dominance at lower temperatures. These findings are in agreement with the conclusions drawn in a previous SMMC calculation [17]. However, we

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also like to mention that the g-extrapolation invoked in previous SMMC studies with the KB3 interaction leads to a slight underestimation of the isovector pair correlations (by about 20% at $T = 2.5$ MeV) as the linear dependence on g, found for $g \leq 0$, i.e. for increased isovector pairing, does not hold for $0 \leq g \leq 1$.

To study the influence of neutron excess on the pairing properties we have finally performed SMMC calculations of ^{60}Ni as a function of temperature. ^{60}Ni differs from its isobar ^{60}Zn by having an extra neutron pair instead of a proton one. The energy expectation value shows the temperature dependence typical for even-even nuclei, similar to ^{60}Zn (Fig. 10). However, the pair correlations, shown in Fig. 11, are rather different than those in ^{60}Zn (see Fig. 7). Both like-nucleon correlations show strong excesses at low temperatures over the mean-field values. At $T = 1$ MeV about half of the excess has vanished, as in other SMMC calculations of even-even nuclei in this mass range. Interestingly the pn correlations, which in the ground state are reduced due to the neutron excess, are roughly constant for $T < 1$ MeV (in fact they even slightly increase when the dominating like-nucleon correlations get weaker). As proposed in Ref. [18] in the presence of a neutron excess the isovector pairing interaction supports the separation of the nuclear system at low temperatures into neutron and proton condensates. At higher temperatures, where the interaction is less important, the isovector pairing correlations follow the ordering of the mean-field values and slowly vanish.

IV. CONCLUSION

We have studied pairing correlations in self-conjugate nuclei in the middle of the pf shell using the pairing plus quadrupole hamiltonian and the SMMC method. Several results of our investigation are noteworthy.

The isovector $J = 0$ pairing correlations show a significant staggering between odd-odd and even-even $N = Z$ nuclei, as noted previously in calculations based on the realistic interaction as well as on a schematic analytically solvable model. While the three isovector channels have identical strengths in even-even $N = Z$ nuclei, the total isovector pairing strength is strongly redistributed in odd-odd self-conjugate nuclei, with a strong enhancement of the proton-neutron correlations.

The importance of isovector proton-neutron correlations decrease drastically if neutrons are added, again in accordance with calculations based on realistic forces and on the analytically solvable model. The additional neutrons increase the coherence among the neutron pair condensate, thus making less neutrons available for isovector proton-neutron correlations. At the same time, the correlations among protons also increase if neutrons are added.

We have studied the temperature dependence of the pairing correlations and of selected observables for ^{54}Co and ^{60}Zn. The even-even $N = Z$ nucleus ^{60}Zn shows the same qualitative trends as other even-even nuclei in this mass region (including the pair breaking transition at temperatures near $T = 1$ MeV). The odd-odd nucleus ^{54}Co has a different behavior. While the proton-proton and neutron-neutron correlations (although much weaker than in even-even nuclei) show a phase transition near $T = 1$ MeV, the dominant $J = 0$ proton-neutron correlations decrease sharply already at lower temperature, and near $T = 1$ MeV become equal to the like-particle correlations. We conjecture that the presence of

low-lying isospin $T = 0$ states in this odd-odd nucleus is responsible for this behavior. The temperature dependence of the isospin expectation value confirms this conjecture. By comparing the isospin expectation values for the schematic Hamiltonian and for the realistic KB3 interaction we conclude that at moderate temperatures pf shell nuclei are dominated by isoscalar correlations. Hence there is a transition from isovector to isoscalar dominance in odd-odd $N = Z$ pf-shell nuclei with increasing temperature. The isoscalar correlations are the focus of work in progress.

ACKNOWLEDGMENTS

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FIGURES

FIG. 1. Pairing correlations $\mathcal{N}_{t_z}$ in the ground states of the $N = Z$ nuclei with masses $A = 46 - 74$. The full lines show the BCS pn correlations, while the dotted lines show the $pp=nn$ correlations. In this and following figures the error bars of the SMMC calculations are indicated. In addition, for $24 \le N \le 30$ the results obtained with the realistic KB3 interaction [10,18] are also shown (not connected by lines to distinguish them).

FIG. 2. Pairing correlations $\mathcal{N}_{t_z}$ in the odd-odd nucleus ^{58}Cu as a function of the scaling λ of the pairing interaction constant. The full lines show the BCS pn correlations, while the dotted lines show the $pp=nn$ correlations.

FIG. 3. Dependence of the expectation value $\langle T^2 \rangle$ (full line) and $\langle J^2 \rangle$ (dashed line) for ^{58}Cu on the scaling λ of the pairing interaction constant. (Only few typical error bars of the quantity $\langle J^2 \rangle$ are shown for clarity.)

FIG. 4. Ground state energies of the $N = Z$ nuclei.

FIG. 5. Pairing correlations $\mathcal{N}_{t_z}$ in the Ni isotopes as a function of the neutron number N. The full line is for pn pairing, the dotted line is for pp pairing, and the dashed-dotted line is for nn pairing. The dotted line with full square points shows the average pairing $(pp + nn + pn)/3$.

FIG. 6. Expectation value $\langle H \rangle$ for ^{54}Co (full line) and ^{60}Zn (dotted line) as a function of temperature.

FIG. 7. Pairing correlations $\mathcal{N}_{t_z}$ in ^{54}Co (part(a), full line for pn, dotted line for $pp = nn$) and for ^{60}Zn (part(b), full line for pn, dotted line for $pp = nn$) as a function of temperature. In both panels the line without points indicates the pairing corresponding to mean field. In that case the pp and pn pairing is essentially identical, and thus only one curve is shown.

FIG. 8. Expectation value of isospin, $\langle T^2 \rangle$, for ^{54}Co (full line) and ^{60}Zn (dotted line) as a function of temperature. The dashed (for ^{54}Co) and dot-dashed (for ^{60}Zn) lines without points indicate the $\langle T^2 \rangle$ values corresponding to mean field. The $\langle T^2 \rangle$ values calculated with the KB3 interaction for temperatures $T > 2.5$ MeV are shown as dotted lines with points; the higher one corresponding to ^{54}Co.

FIG. 9. Expectation value of angular momentum, $\langle J^2 \rangle$, for ^{54}Co (full line) and ^{60}Zn (dotted line) as a function of temperature. The mean field values are shown as the long-dashed line for ^{54}Co and the double-dotted line for ^{60}Zn.

FIG. 10. Expectation value $\langle H \rangle$ for ^{60}Ni as a function of temperature.

FIG. 11. Pairing correlations $\mathcal{N}_{t_z}$ in ^{60}Ni as a function of temperature. The full line shows the pn correlations, the dotted line the pp correlations, and the dot-dashed line the nn correlations.